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Checkerboard patterns in the t-J model

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Using the density matrix renormalization group, we study the possibility of real space checkerboard patterns arising as the ground states of the t-J model. We find that checkerboards with a commensurate (π,π) background are not low energy states and can only be stabilized with large external potentials. However, we find that striped states with charge density waves along the stripes can form approximate checkerboard patterns. These states can be stabilized with a very weak external field aligning and pinning the CDWs on different stripes.

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Scanning tunneling microscopy (STM) studies have reported checkerboard-like modulation patterns in the tunneling conductance of optimally doped $Bi_2Sr_2CaCu_2O_{8+\delta}$ (Bi2212) near vortex cores [1] and in nearly optimally doped Bi2212 in the absence of an external field [2]. Checkerboard modulations have also been found in underdoped Bi2212 [3, 4] in the pseudogap region, and in lightly doped $Ca_{2-x}Na_xCuO_2Cl_2$. These modulations were found to be oriented along the Cu-O axes. In the vortex case [1], the tunneling conductance was modulated on a length scale of order $4.3a$, where a is the Cu-Cu spacing. Some degree of one-dimensionality was observed with one Cu-O direction exhibiting a stronger spectral intensity than the other. In their zero field studies of Bi2212, Howald, et. al. [2] interpreted their STM measurements in terms of a two-dimensional system of stripes with a charge modulation of $4a$. They noted that while the modulation appeared "almost checkerboard-like", the defect structure suggested that the underlying order was one-dimensional.

In experiments on underdoped Bi2212 by Vershinsin *et. al* [3], the modulation length was $4.7a \pm .2a$ and appeared only in the normal phase at bias voltages less than a pseudogap energy of order 35 meV. In this case the observed conductance pattern appeared to be inherently two-dimensional, suggesting an absence of static stripes but leaving open the possibility of fluctuating stripes. In the low temperature STM studies of McElroy *et. al* [4], a checkerboard pattern with a spacing of order $4.5a$ was observed, which appeared in the underdoped nanoscale pseudogap regions at bias voltages ~ 60 meV. In $Ca_{2-x}Na_xCuO_2Cl_2$[5], a commensurate $4a \times 4a$ checkerboard with an additional complex incommensurate $4a/3 \times 4a/3$ internal pattern has been observed in the pseudogap regime. In these experiments, the conductance patterns showed no significant breaking of 90° rotational symmetry, suggesting a two-dimensional checkerboard pattern as opposed to a striped pattern.

Although differing in detail, these measurements provide evidence of an electronic locally-ordered phase which appears when the $d_{x^2-y^2}$ superconducting phase is suppressed. Various suggestions for this electronic phase have been put forth but at present its nature remains unclear. Several of these involve charge density waves. Chen *et. al* [6, 7] have mapped a Hubbard model with extended Coulomb interactions onto an effective bosonic SO(5) model and find a phase with a checkerboard density of d-wave Cooper pairs. Anderson [8] has proposed a 4×4 structure consisting of a Wigner solid of hole pairs embedded in a sea of d-wave spin singlet pairs. Fu *et. al* [9] have used a Slater determinant variational ansatz to approximate the groundstate of a generalized Hubbard model with Coulomb and near-neighbor exchange interactions. They find that a soliton hole crystal phase can form with a modulation length which is $\sqrt{2}$ times that of the d-wave pair field CDW of Chen *et. al* and Anderson. Both Chen and Fu proposed charge density phases coexisting with a background spin state which has commensurate $Q = (\pi, \pi)$ antiferromagnetic order. Chen *et. al* note that in principle this is not an intrinsic feature of their approach, but that the stability of an incommensurate magnetic state would require extended magnetic interactions which have not been included in their study.

Here we investigate the possibility of checkerboard order as a low energy phase of the 2D t-J model using the density matrix renormalization group (DMRG)[10]. Our previous work using DMRG has shown the presence of striped phases as the ground state of large t-J clusters[11]. However, these states are sensitive to boundary conditions and to additonal terms in the Hamiltonian[12]. It is possible that a checkerboard phase could be stabilized with appropriate boundary conditions or small additional terms.

It is important to specify what is meant by a checker-

board phase. The simplest possibility, which has been the principle focus of some of the previous theoretical work, consists of pairs of holes living primarily on 2×2 placquettes, arranged in a checkerboard pattern. The spin background in between has commensurate antiferromagnetism. Here one imagines that an attraction between the holes has formed the pairs, but that these pairs repel each other, forming a Wigner crystal-like state. In this scenario the interaction between the pairs is something more complicated than an isotropic repulsion, so that a checkerboard pattern results rather than a triangular lattice of pairs. We call this phase the isotropic checkerboard phase (ICB).

Another possibility assumes that the dominant instability is stripe order. However, as has been observed previously in simulations, along each stripe there is a tendency for CDW order, associated with localized pairs in the stripe. To make an approximate checkerboard pattern, one could imagine that the CDW along each stripe is pinned, and furthermore that due to lattice or interlayer effects the CDWs on the different stripes line up. This pattern would show two types of anisotropy: first, the spin background would have the usual striped π-phase shifted antiferromagnetic arrangement. Second, the charge density pattern would be more strongly modulated perpendicular to the stripes. This pattern could look like an ICB phase in an STM measurement, which would not detect the spin pattern, if the anisotropy were weak. We call this phase the stripe checkerboard phase (SCB).

Note that there is a third possibility, stemming from dynamic stripes. Here one could imagine that the orientational order of the stripes fluctuates, with large domains rotating by 90°. Since the STM measurements are made over long time scales, they would yield a superposition of the two orientations. To get a checkerboard pattern one would assume that the transverse translational motion of the stripes is pinned. A difficulty with this approach is that the pinning potential must be simultaneously weak enough to allow orientational fluctuations and strong enough to pin translational motion. As discussed below, our DMRG results for the t-J model in the parameter range we have studied show no tendency towards fluctuating orientational order.

To study the stability of an ICB phase, we use to our advantage a weakness of DMRG, namely that a DMRG simulation, keeping a finite number of states, can get stuck in a metastable ground state. For example, if on a particular cluster a striped state oriented in the x-direction has slightly lower energy than a y oriented stripe state, but we prepare the system in the y oriented state, we may not see, even after dozens of sweeps, the transition to the x-orientation. Here, we apply external fields to stabilize an ICB state, and then remove the fields and observe the results. In Fig. 1 we show results for a 10×8 t-J cluster with $J/t = 0.35$, 8 holes, and cylindrical

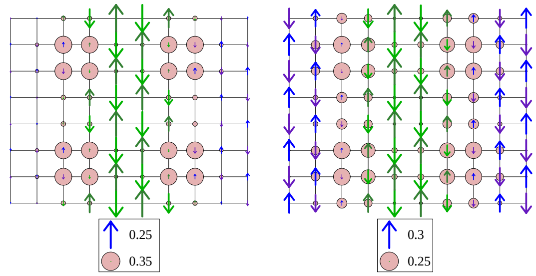

FIG. 1: Charge and spin configurations of a t-J model in a pinned checkerboard configuration. The results show the expectation value of $< S_z >$ and $< n_h >$ for a 10x8 t-J cluster with cylindrical boundary conditions: open in x, periodic in y. Here there are 8 holes and J/t = 0.35. Initially, a local pinning potential of -0.5 t was placed on the 16 sites making up 4 the placquettes visible in the left panel. Nine sweeps were performed, keeping up to $m = 1000$ states, with the result shown in the left panel. Subsequently, the pinning potential was turned off. In the right panel, we show the result after three more sweeps were performed, reaching m=1500 states.

boundary conditions. The left panel shows the ICB state stabilized by a local pinning potential $-0.5t(n_{i\uparrow}+n_{i\downarrow})$ on the 16 sites i making up the four placquettes visible in the figure. The left panel is the state after 9 DMRG sweeps, keeping up to m=1000 states. Note that even with the strong pinning potential, the motion of the holes has considerably weakened the antiferromagnetism between the placquettes. In the right panel, we show the result of the same simulation after the pinning potential was removed and three more sweeps were performed, reaching m=1500 states. Within one sweep of releasing the pinning, the π phase shifts characteristic of the stripe phase form. Also, the hole density spreads out in the y-direction almost as quickly. We continued this run up to 17 sweeps and 3000 states. There was very little difference between the final configuration and that shown in the right panel. Results from other runs with different cluster sizes and boundary conditions yield consistent results: the ICB phase does not appear even as a metastable ground state. Systems prepared in an ICB state immediately decay to an SCB ground state.

However, from this we cannot conclude that the SCB state is the ground state. In particular, the fact that the CDWs along the two stripes in the right panel are lined up may be a residual effect of the initial ICB state. In Fig. 2 we show results for two simulations differing from Fig. 1 only in pinning potentials. In each case, the initial ICB pinning potentials were not applied; instead, two sites were given permanent pinning local potentials. In the left panel, the two pinning sites were aligned (large circles), while in the left, they were antialigned. The lower plot shows the total energies of the systems as a function of the number of states kept per block as DMRG sweeps were performed on the systems. There is no sig-

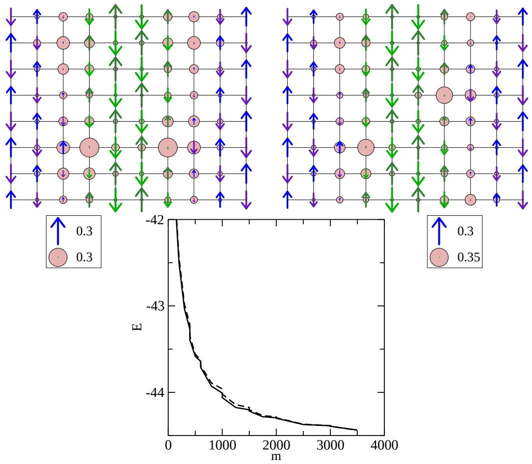

FIG. 2: Charge and spin configurations of a t-J cluster with two sites pinned with a local potential of $-0.5t$. In each panel, the sites pinned have the large circles. The lower plot shows the total energies of the systems as a function of the number of states kept per block as DMRG sweeps were performed on the systems.

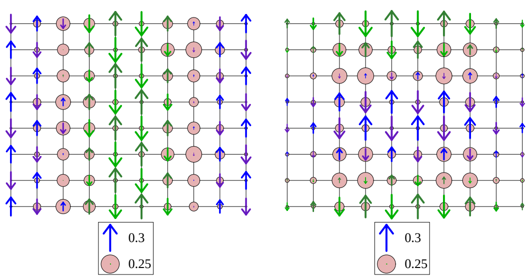

FIG. 3: Charge and spin configurations with different values of the exchange coupling linking vertical and horizontal bonds. In both cases $J_x = 0.35$. In the left panel, $J_y = 0.37$, and in the right, $J_y = 0.38$.

nificant detectable difference in the total energies of the two configurations. In fact, it seems more likely that the CDWs on adjacent stripes would be antialigned. First, we know from previous DMRG studies that stripes repel each other, and the simplest explanation is a Fermi repulsion between the holes in the transverse tails of the stripes. A CDW along a stripe would modulate this hole density, making it look like the width of the stripe varied along its length. In order to minimize the Fermi repulsion, we expect antialignment of the CDWs. Second, the longer range Coulomb repulsion terms left out of the t-J model would certainly favor this.

We now consider external potentials which could stabilize a checkerboard pattern. The ICB phase appears sufficiently unstable that it would require an unphysically large stabilizing potential. The SCB phase, in contrast, is stabilized by a weak potential, which could

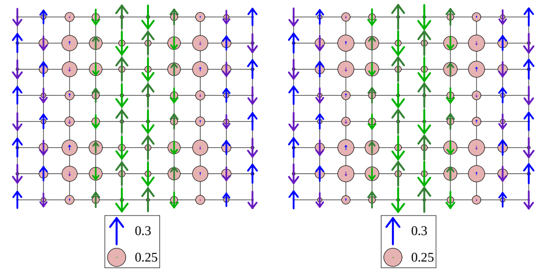

FIG. 4: Charge and spin configurations with a local field in a pattern transverse to the stripes applied. In the simulation shown in the left (right) panel, potentials of -0.05t (-0.1t) were applied to four of the horizontal rows of sites: rows 2,3,6, and 7.

be generated by interlayer effects or small lattice distortions. For example, the tilt distortion in the LTT phase of La$_{1.6-x}$Nd$_0$.4Sr$_x$CuO is known to pin stripes. This may occur due to Coulomb interactions, or, as discussed by Kampf, et. al[13], because of an anisotropic exchange interaction which arises naturally from the lattice tilt distortion. For example, in Fig. 3, we show the result of increasing the exchange coupling in the (spatial) y direction J_y slightly. For the isotropic case, the periodic boundary condtions in the y direction favor vertical stripes. For $J_x = 0.35$, this orientation persists up to about $J_y = 0.37$ (left panel). However, for $J_y = 0.38$, horizontal stripes have lower energy in the 10×8 cluster, as seen in the right panel. The transition between the orientation seems rather sharp; there does not appear to be any finite intermediate isotropic region, corresponding to fluctuating orientational order. However, one cannot draw a general conclusion from this result: other models, including Hubbard or extended t-J models, may show different results. Note that in the present case the reorientation of the stripes required only a very small change in J_x/J_y. Note also that an SCB pattern has appeared in the right panel. In this case, the open boundaries on the left and right pin and align the CDWs along each stripe.

Now consider the response of the system to a weak potential with a bond centered spatial modulation with $Q = (0, 2\pi/4a)$. Such a potential would be expected to arise, for example, from the Coulomb interactions due to an adjacent layer in which the stripe orientation was rotated by 90°. In Fig. 4 we show results from a system similar to those of Fig. 1 and 2, but with this type of applied field. In the left panel, potentials of -0.05t were applied to four of the horizontal rows of sites: rows 2,3,6, and 7, with no potentials on the other rows. In the right panel, we applied a potential of $-0.1t$. We see that a rather modest field is sufficient to stabilize the SCB pattern.

In order to study the response of a stripe to a CDW inducing field with higher precision, we consider a two

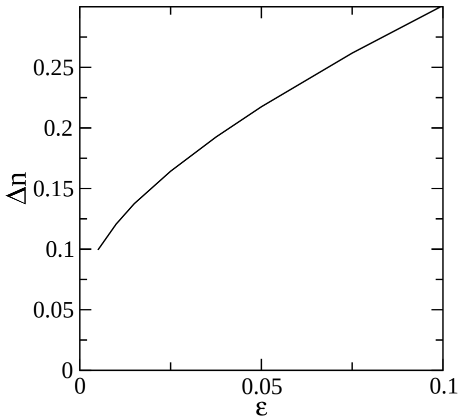

FIG. 5: Charge density wave response to an applied local potential on a two leg t-J ladder, with doping 0.25. The applied field had periodicity 4 with rungs 1 and 2 with $+\epsilon$, rows 3 and 4 $-\epsilon$, etc. The measured response Δn is the absolute difference in hole densities between sites 2n and 2n+1.

leg ladder as a model of a bond centered stripe. As is well known, DMRG is extremely accurate on single chain and two leg ladder systems. Here we apply a potential ϵ and measure the response Δn in the central region of a 64×2 ladder, with a doping of 0.25 and $J/t = 0.35$. In a two-leg ladder[14], CDW and pairing correlations have competing power law decays. Because of the power law decay, we expect a diverging susceptibility for a CDW inducing potential. Here we are concerned more with the size of the response to a finite potential than the limit as the potential tends to zero. The results are shown in Fig. 5. We see that even a weak potential induces a strong CDW response.

In summary, a real space checkerboard pattern with an antiferromagnetic spin background does not appear to be a low energy state of the t-J model. Instead, striped states with CDWs along the stripes can give approximate checkerboard patterns, but an external field, possibly arising from lattice distortions and interplane Coulomb interations, appears necessary to align the CDWs in each stripe.

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